

FIG. 1(a)

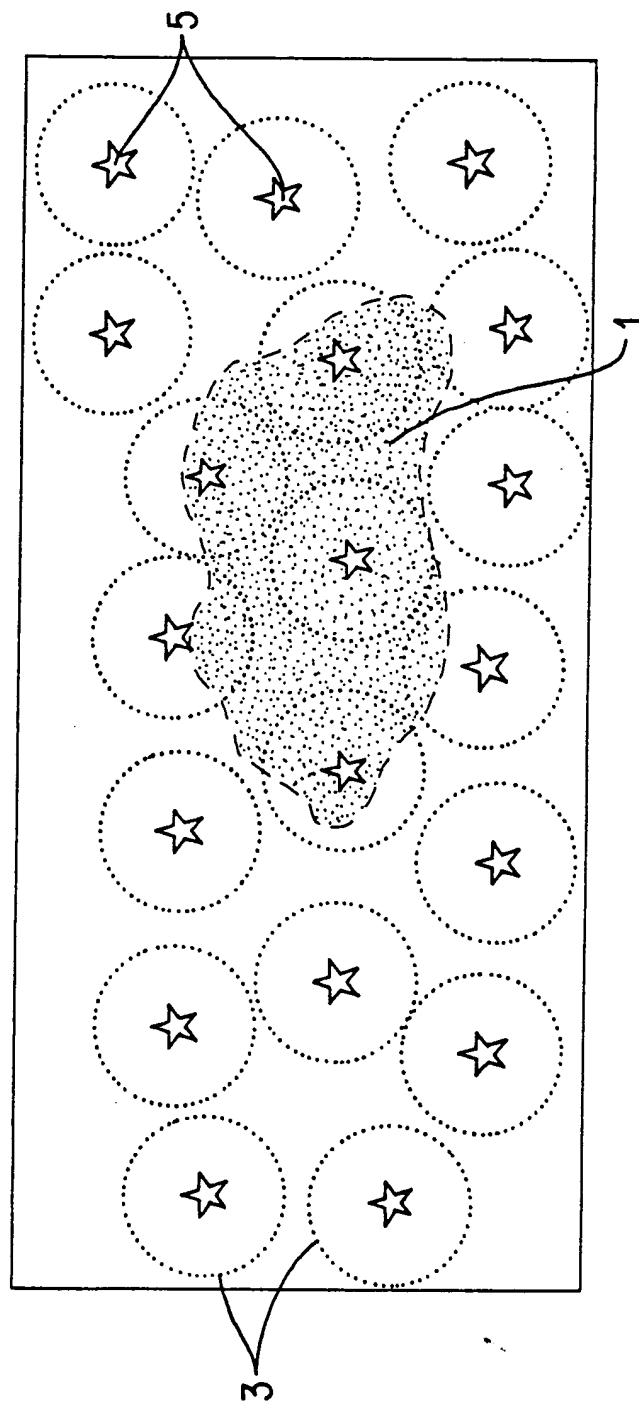


FIG.1(b)

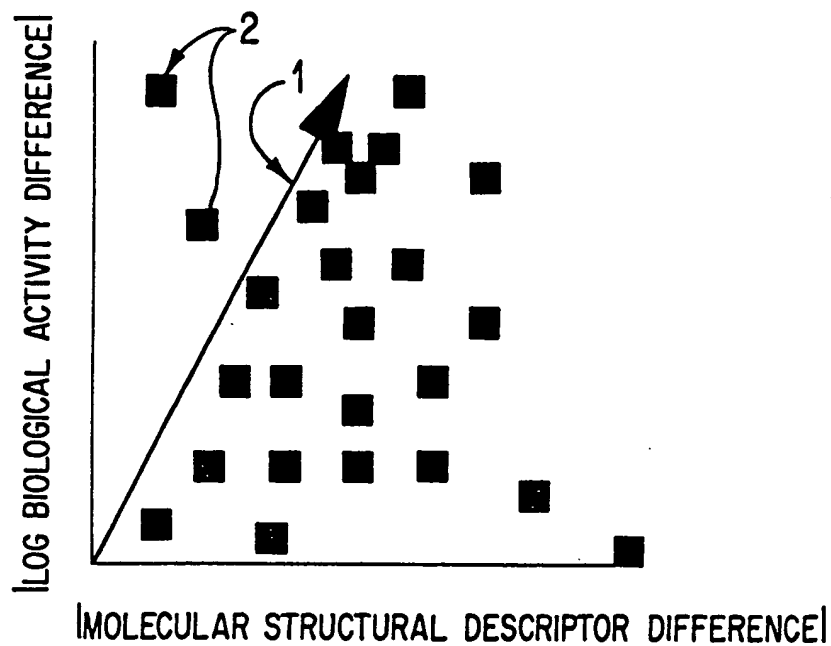


FIG. 2

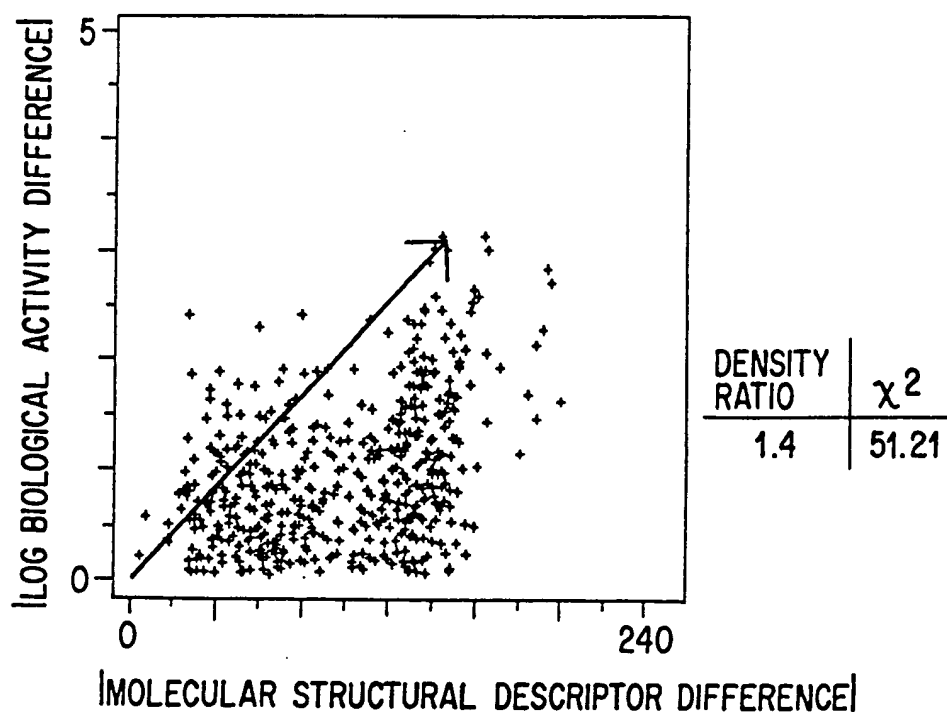


FIG. 3

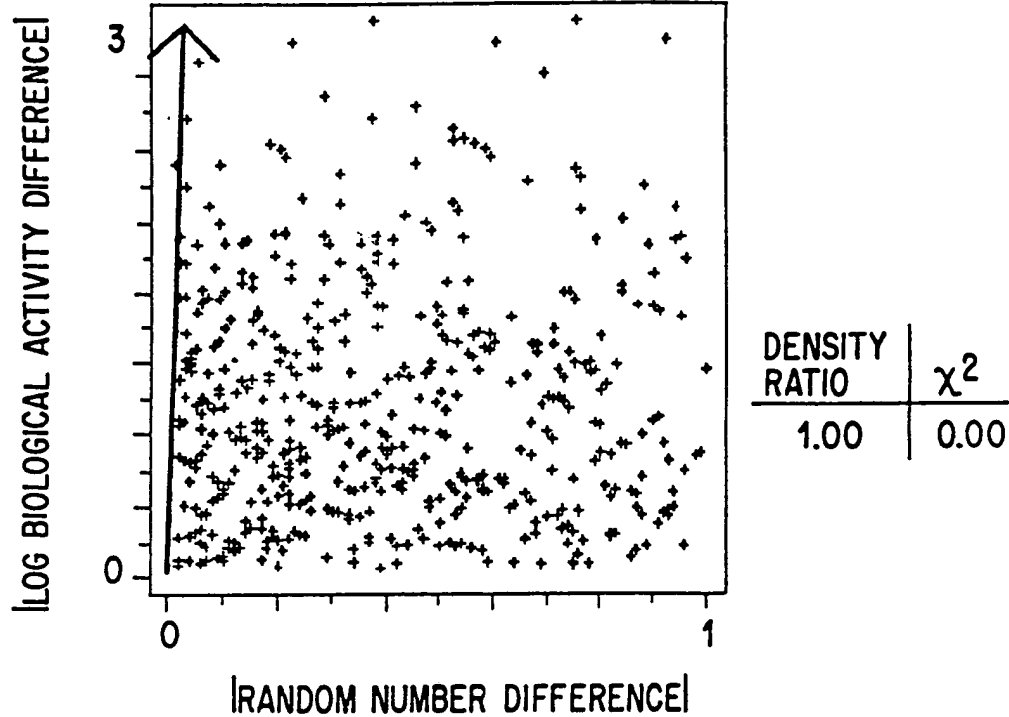


FIG. 4

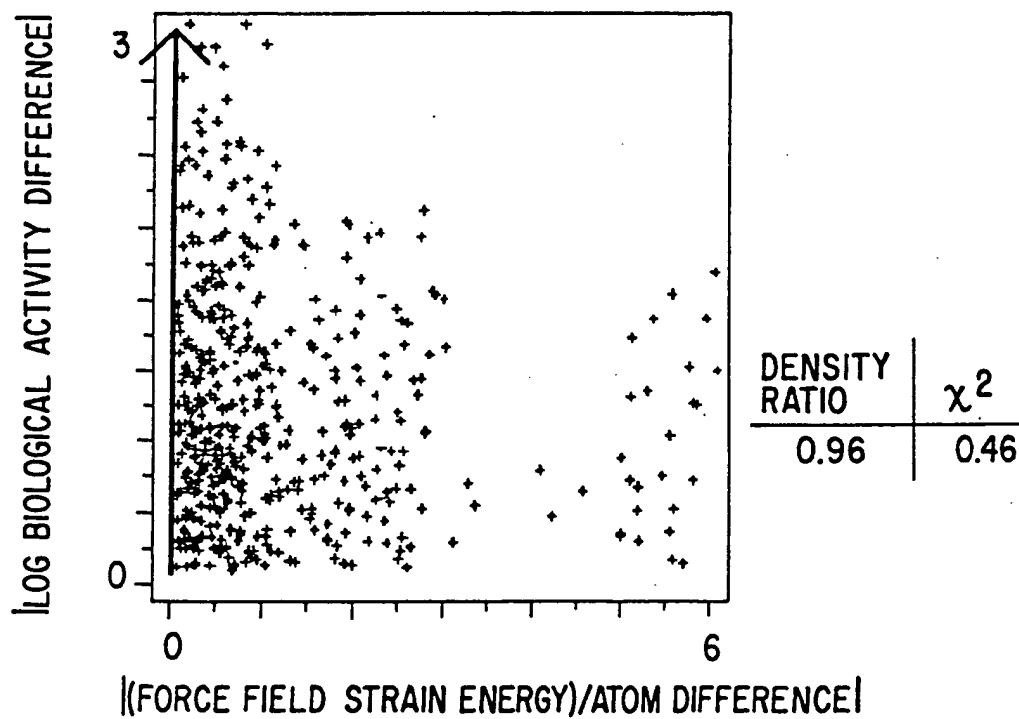
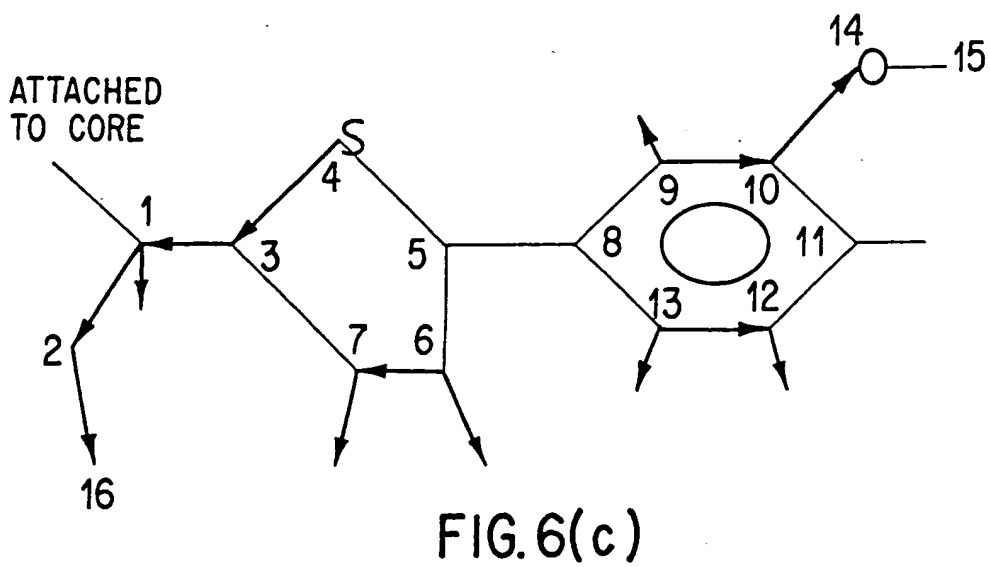
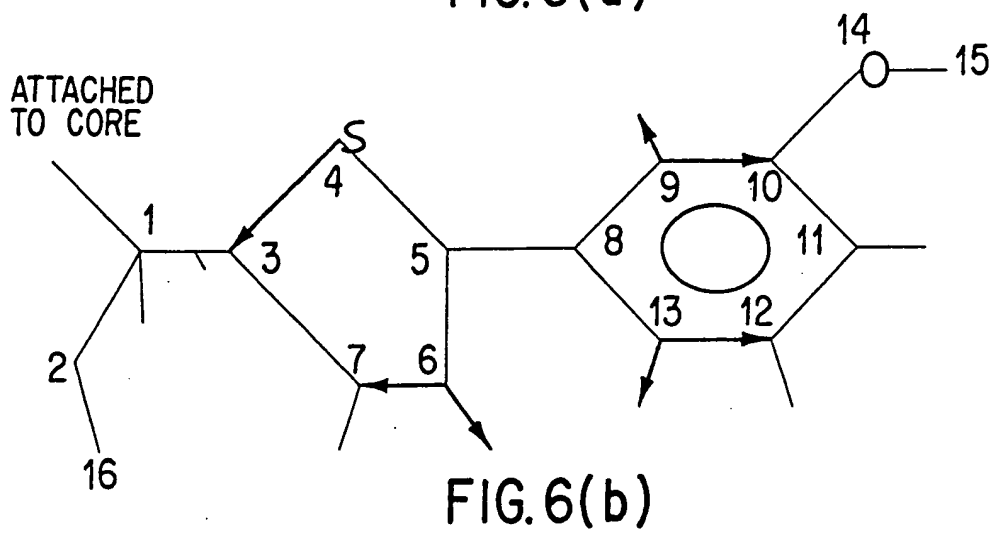
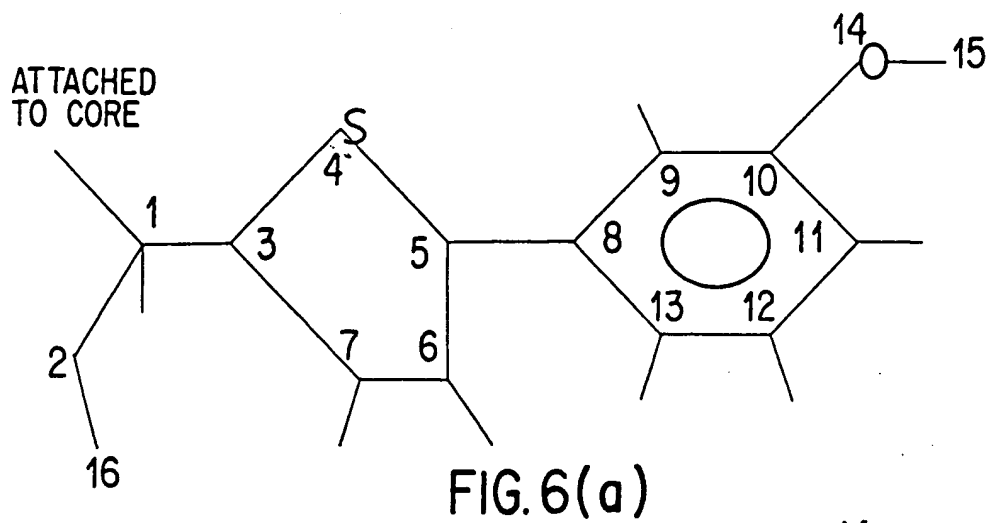


FIG. 5



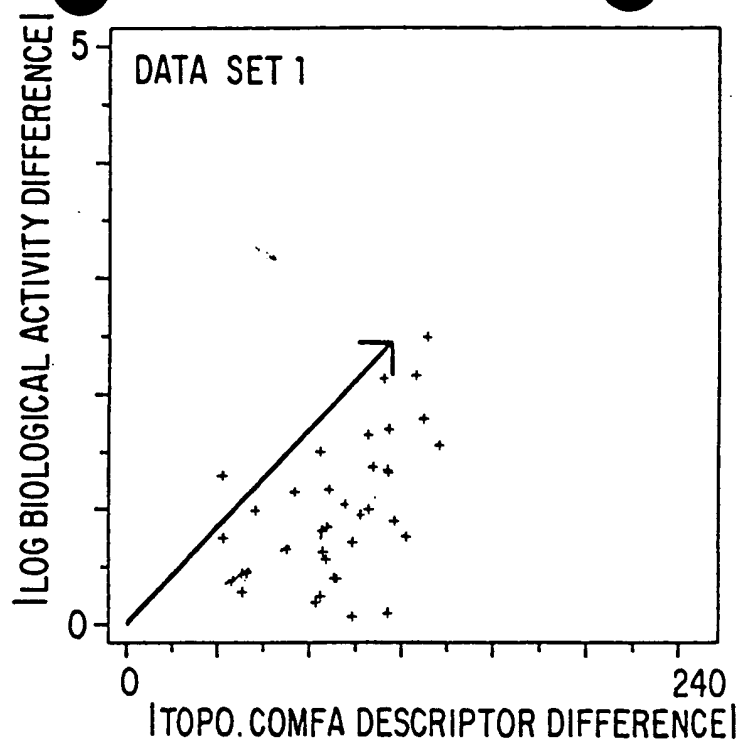


FIG.7(a)

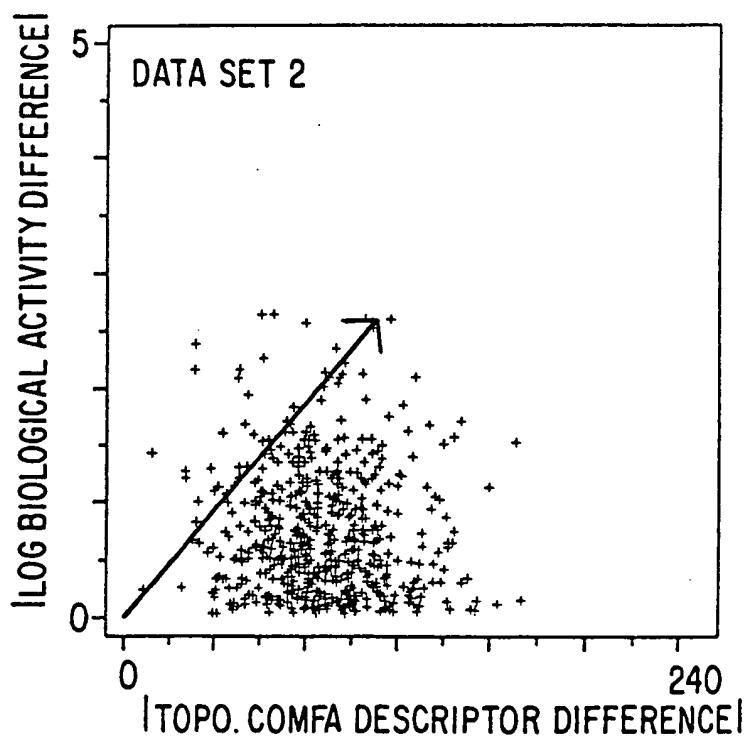


FIG.7(b)

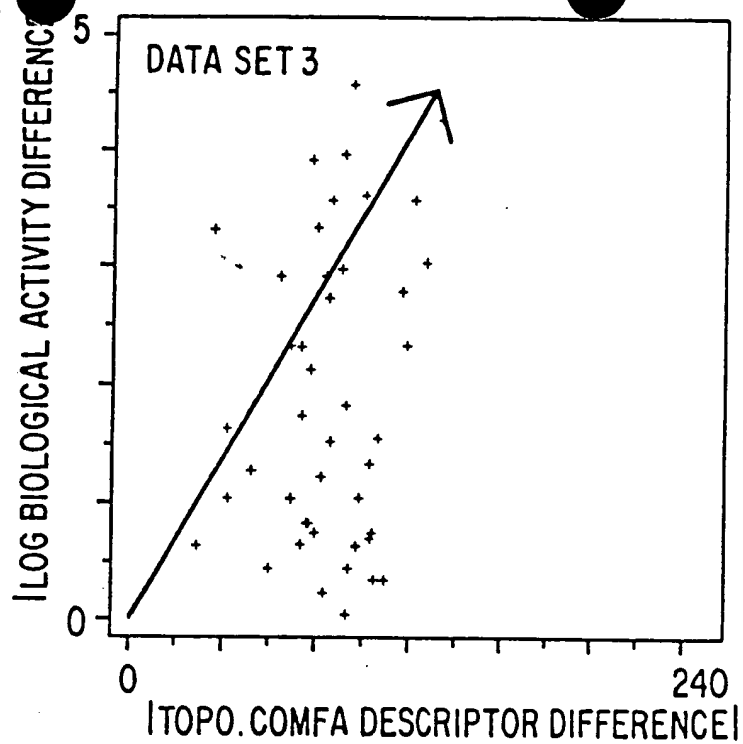


FIG. 7(c)

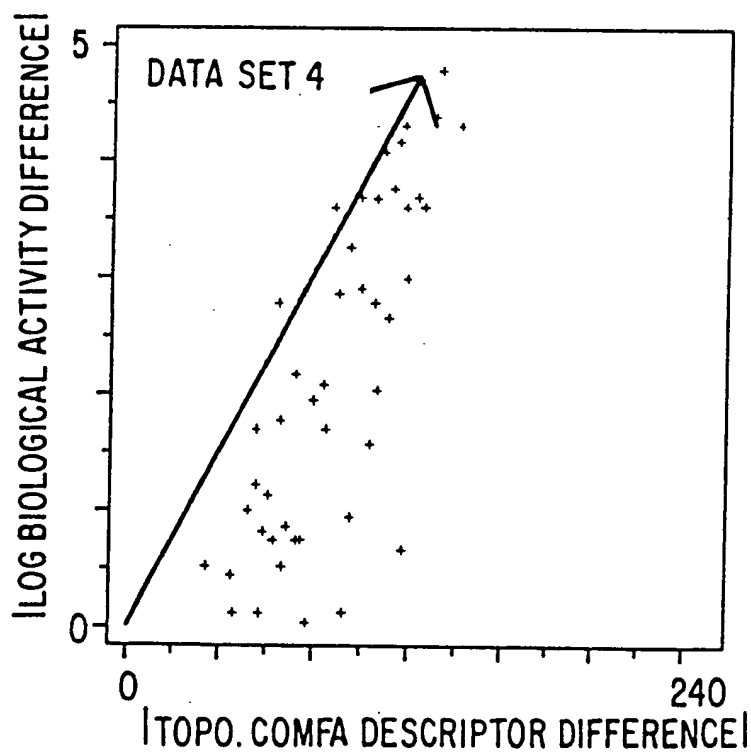


FIG. 7(d)

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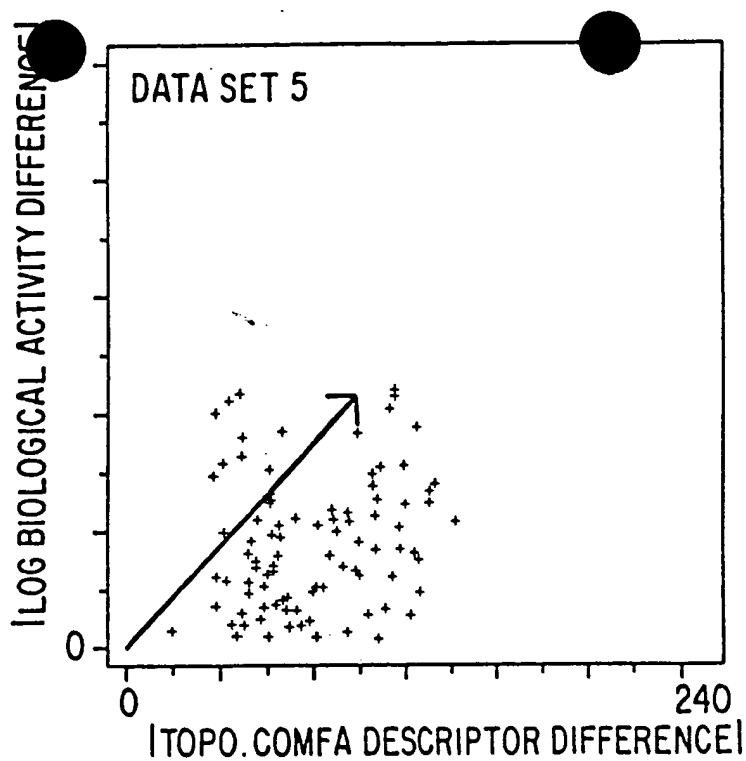


FIG.7(e)

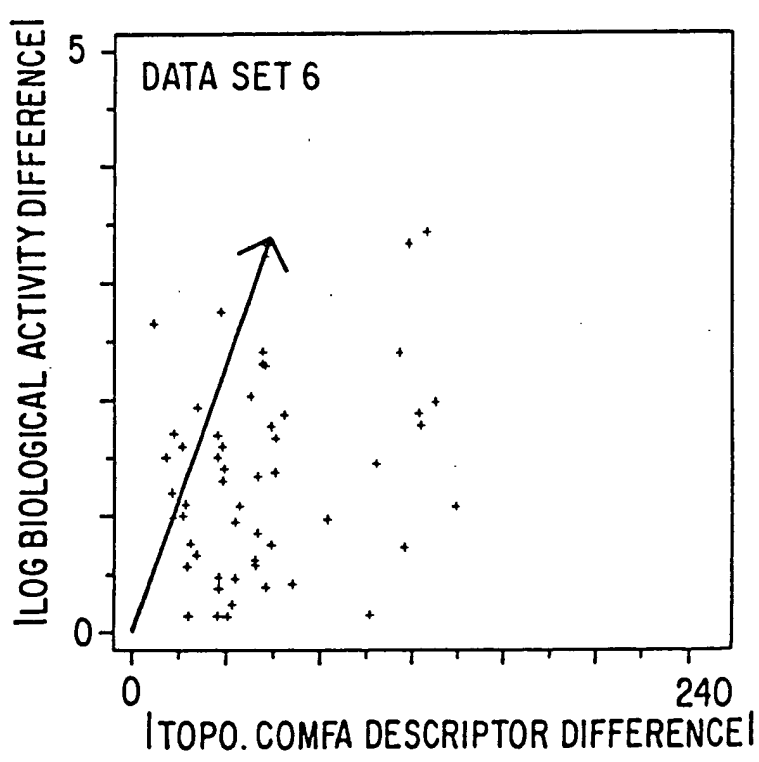


FIG.7(f)

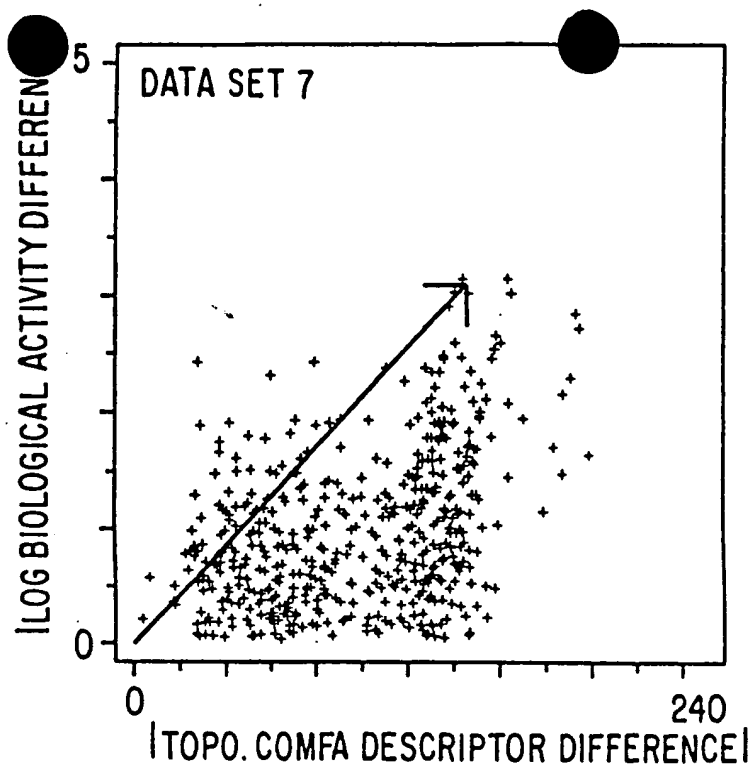


FIG.7(g)

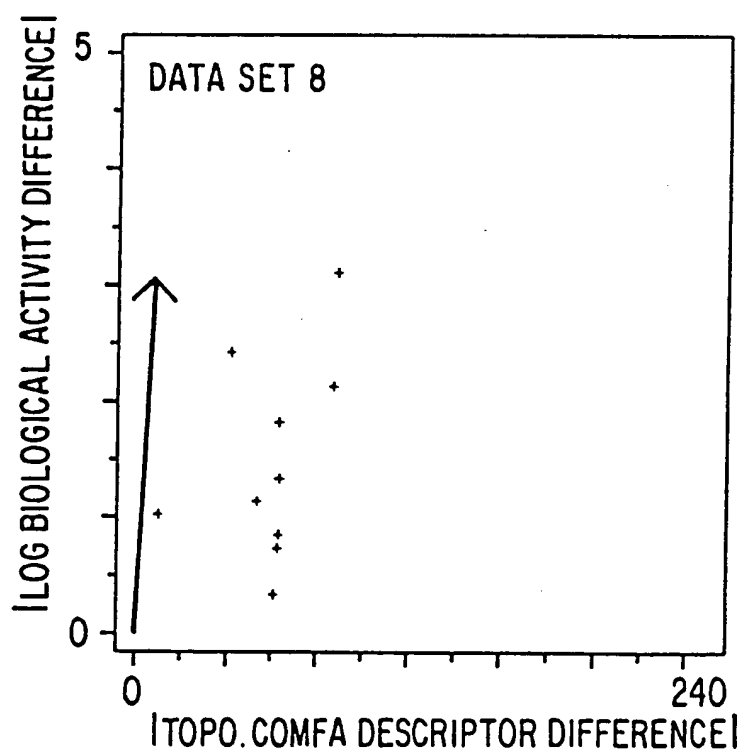


FIG.7(h)

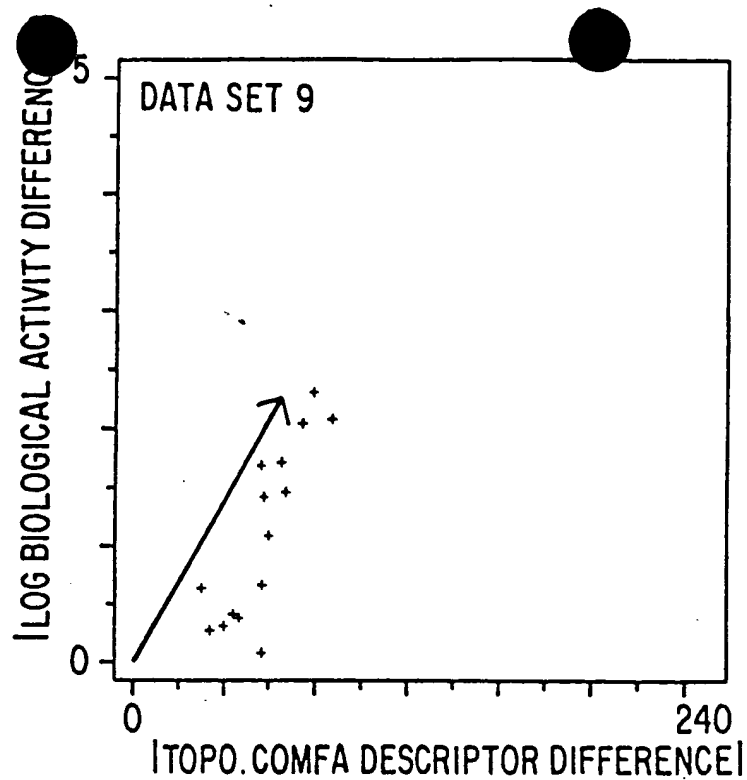


FIG.7(i)

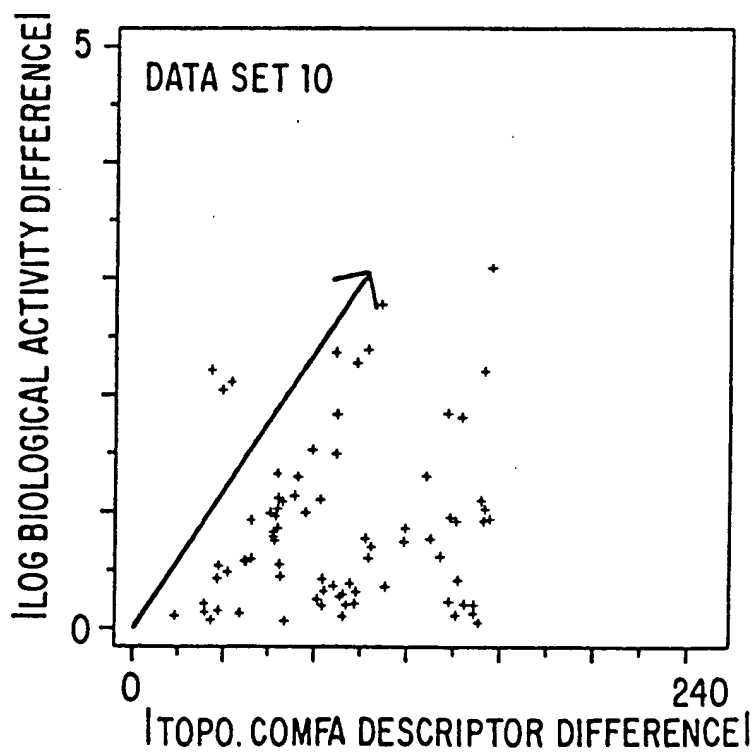


FIG.7(j)

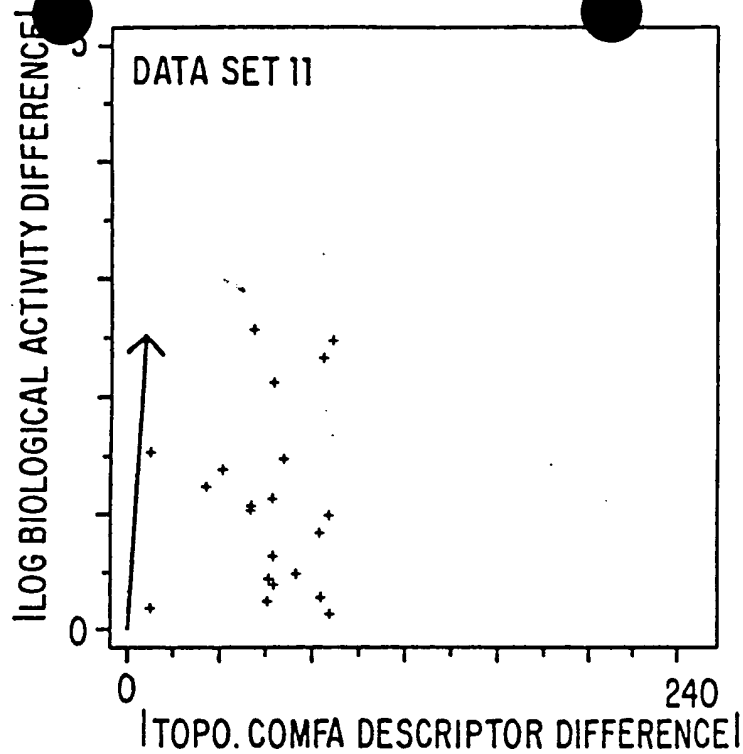


FIG.7(k)

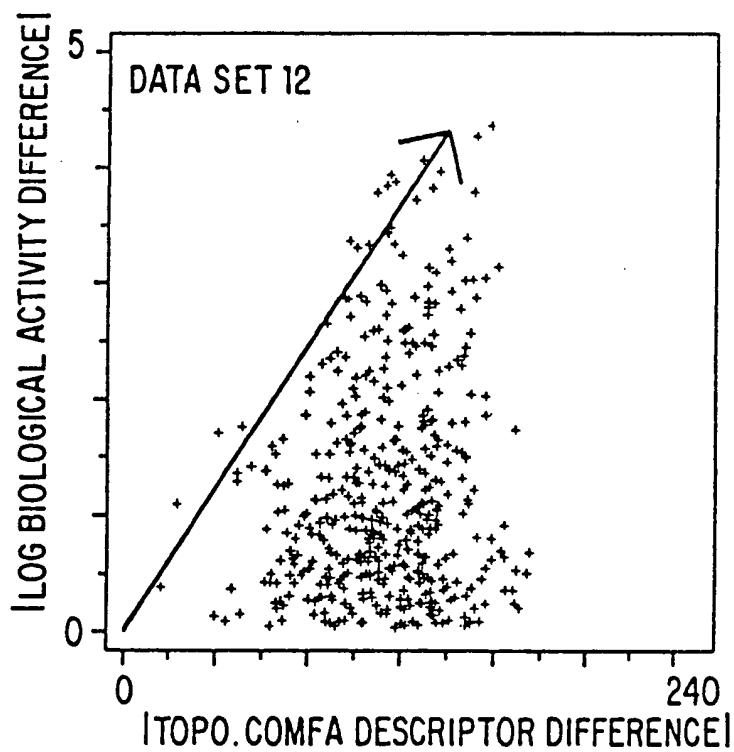


FIG.7(l)

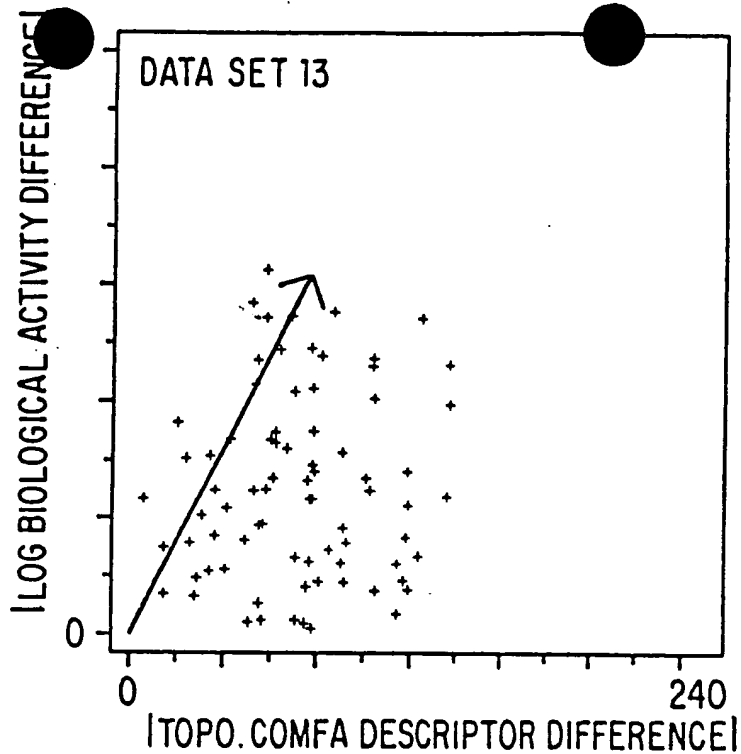


FIG.7(m)

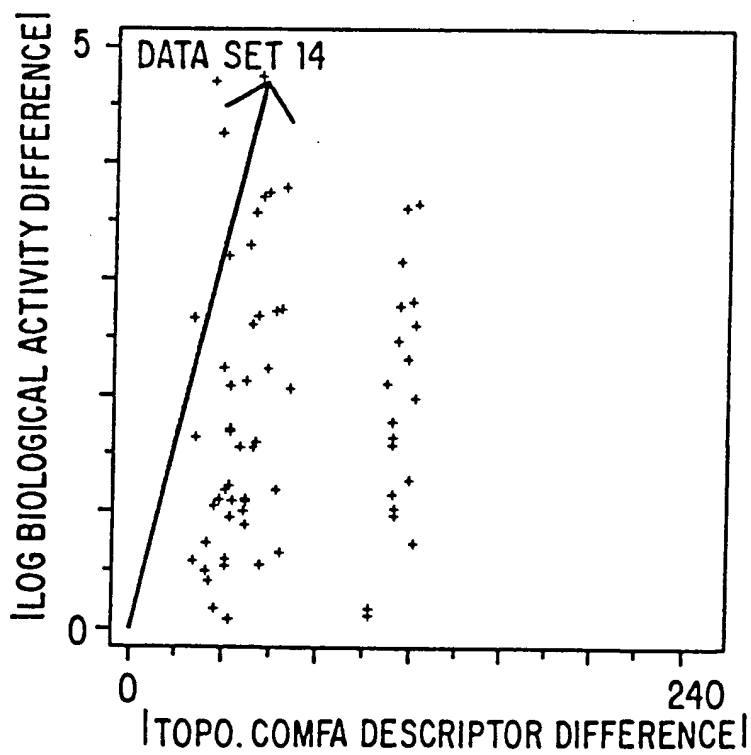


FIG.7(n)

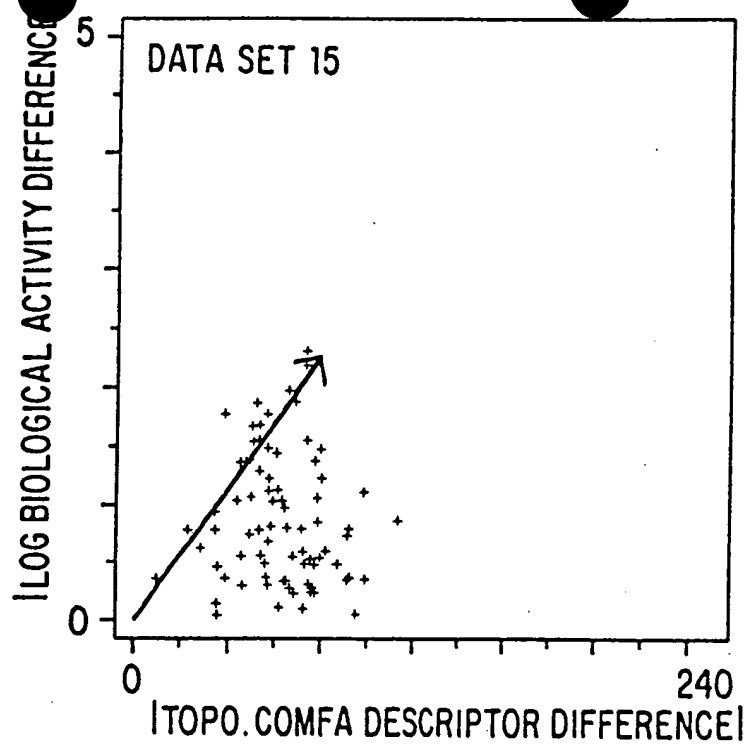


FIG.7(o)

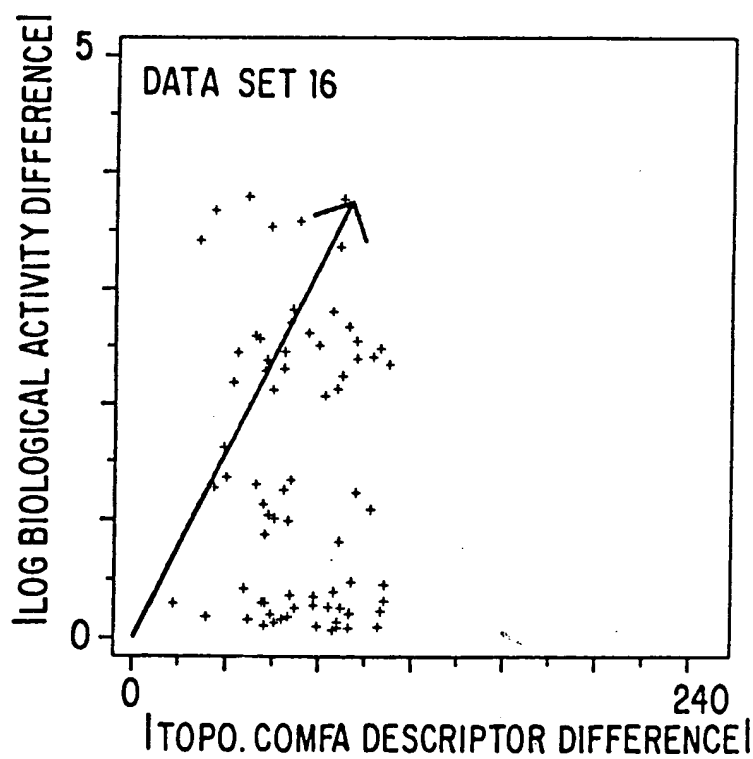


FIG.7(p)

FOUO 80292260

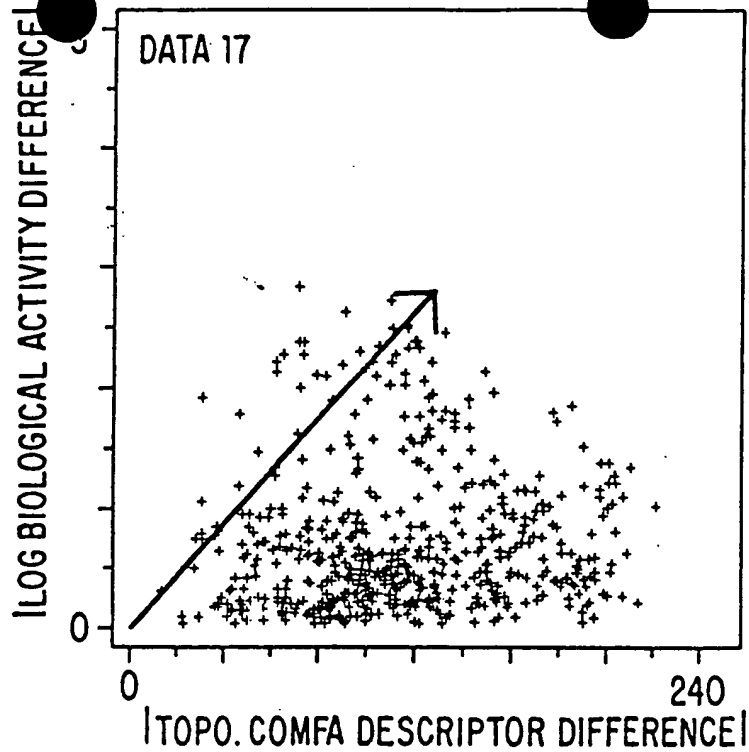


FIG.7(q)

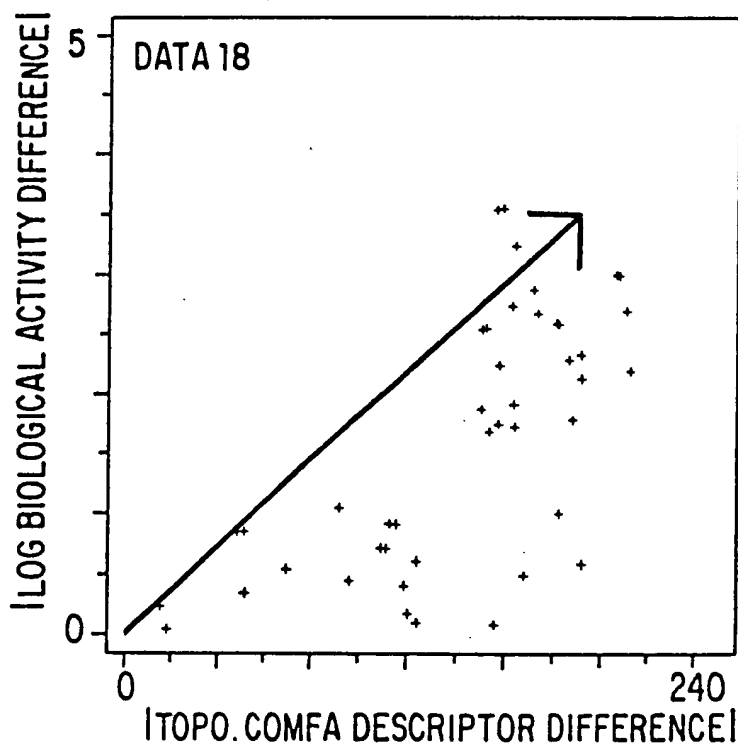


FIG.7(r)

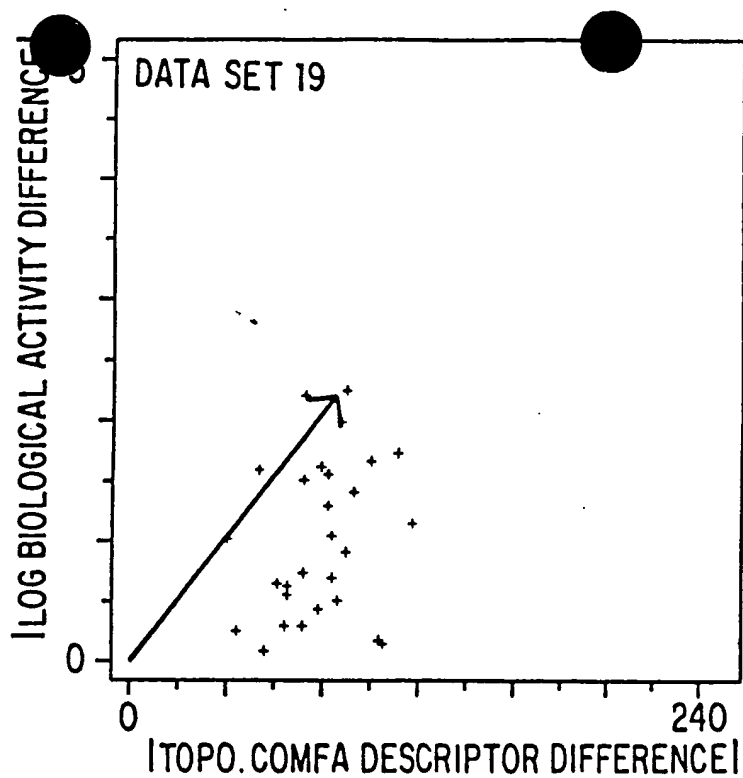


FIG.7(s)

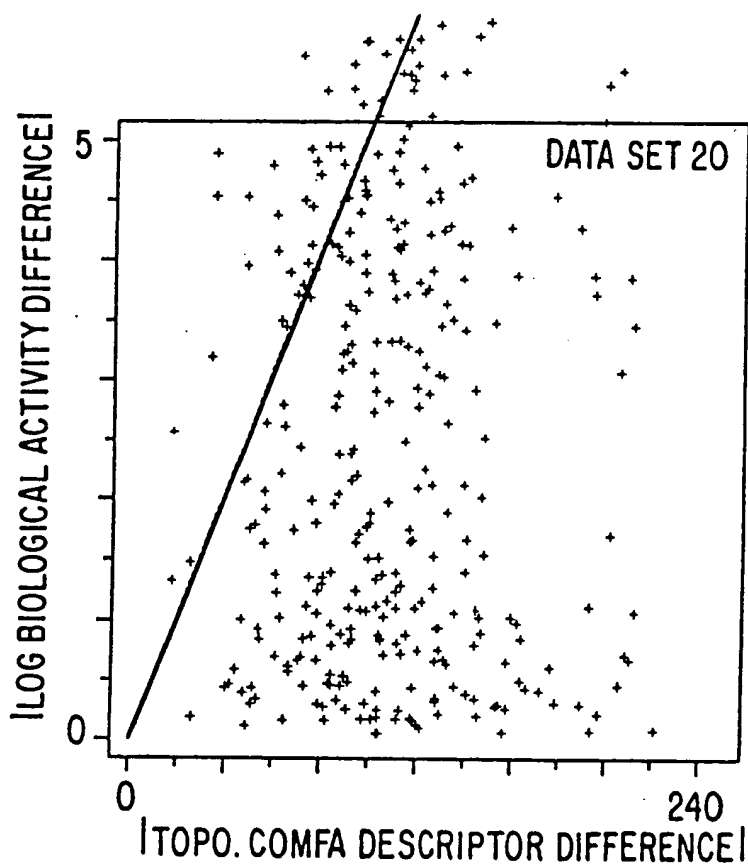
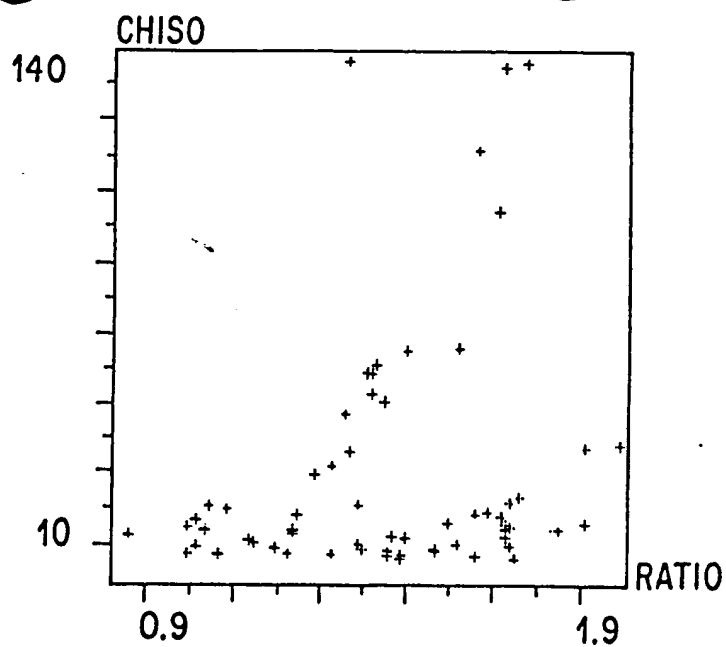


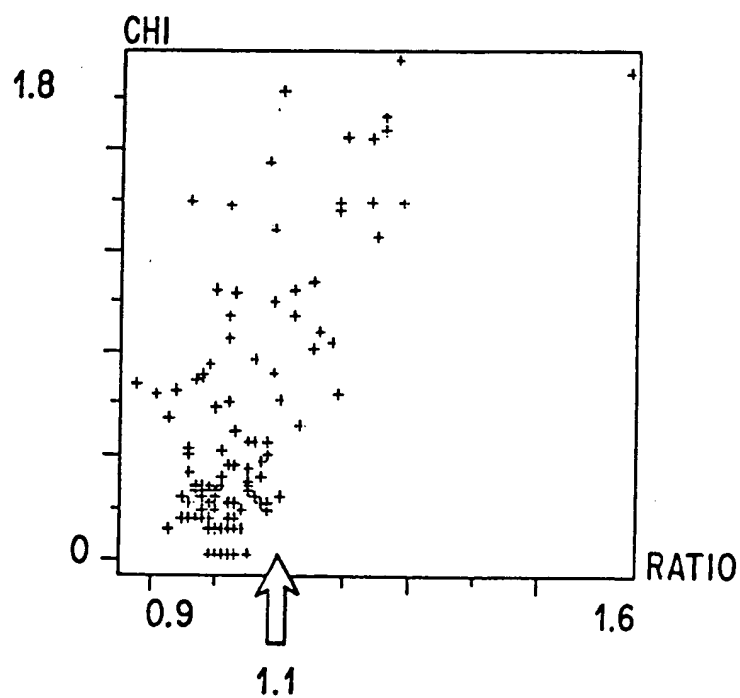
FIG.7(t)

105020" 80232260



1.1

FIG. 8(a)



1.1

FIG. 8(b)

FOUO 30494260

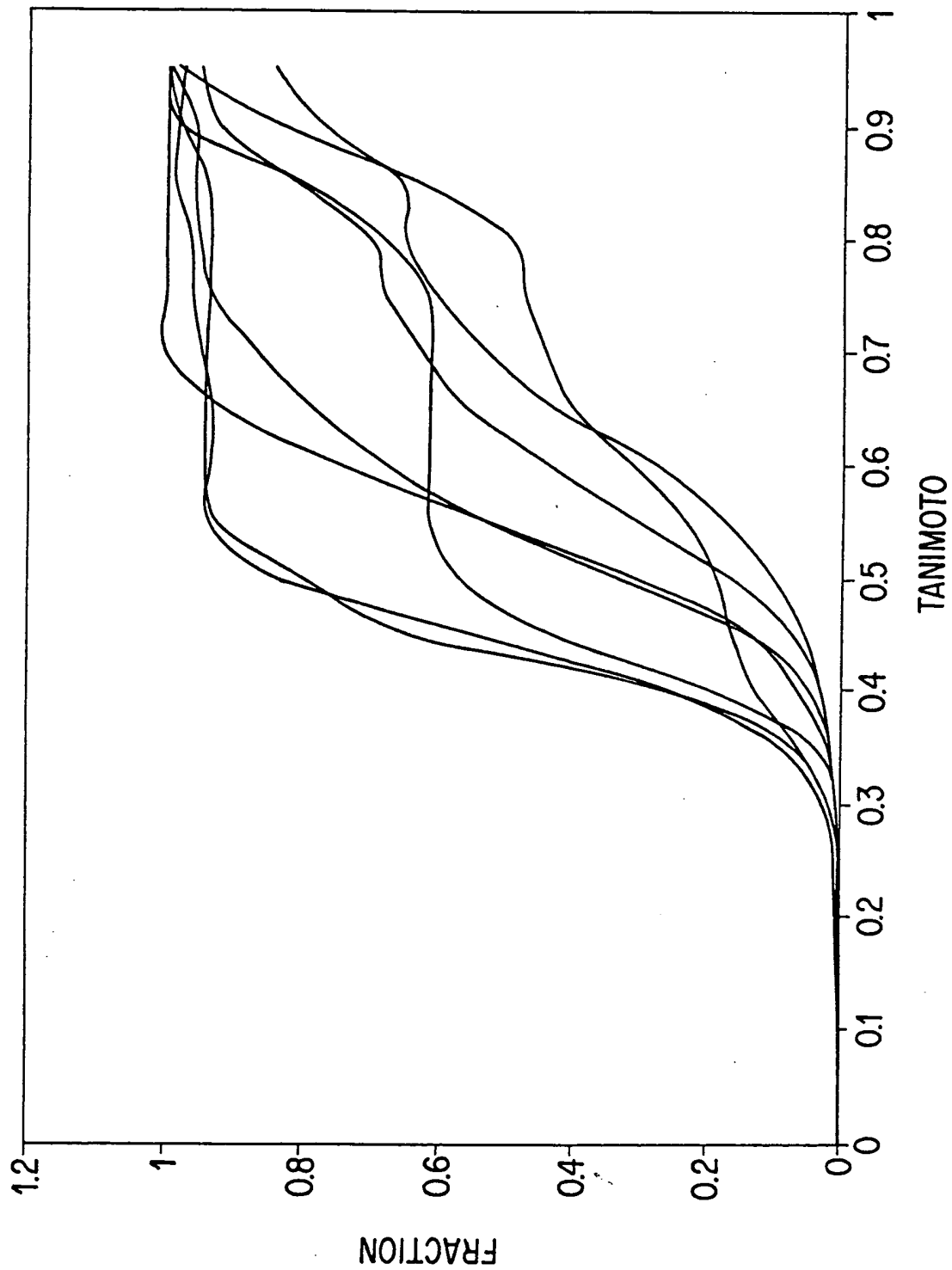


FIG. 9(a)

FO9020" 8029260

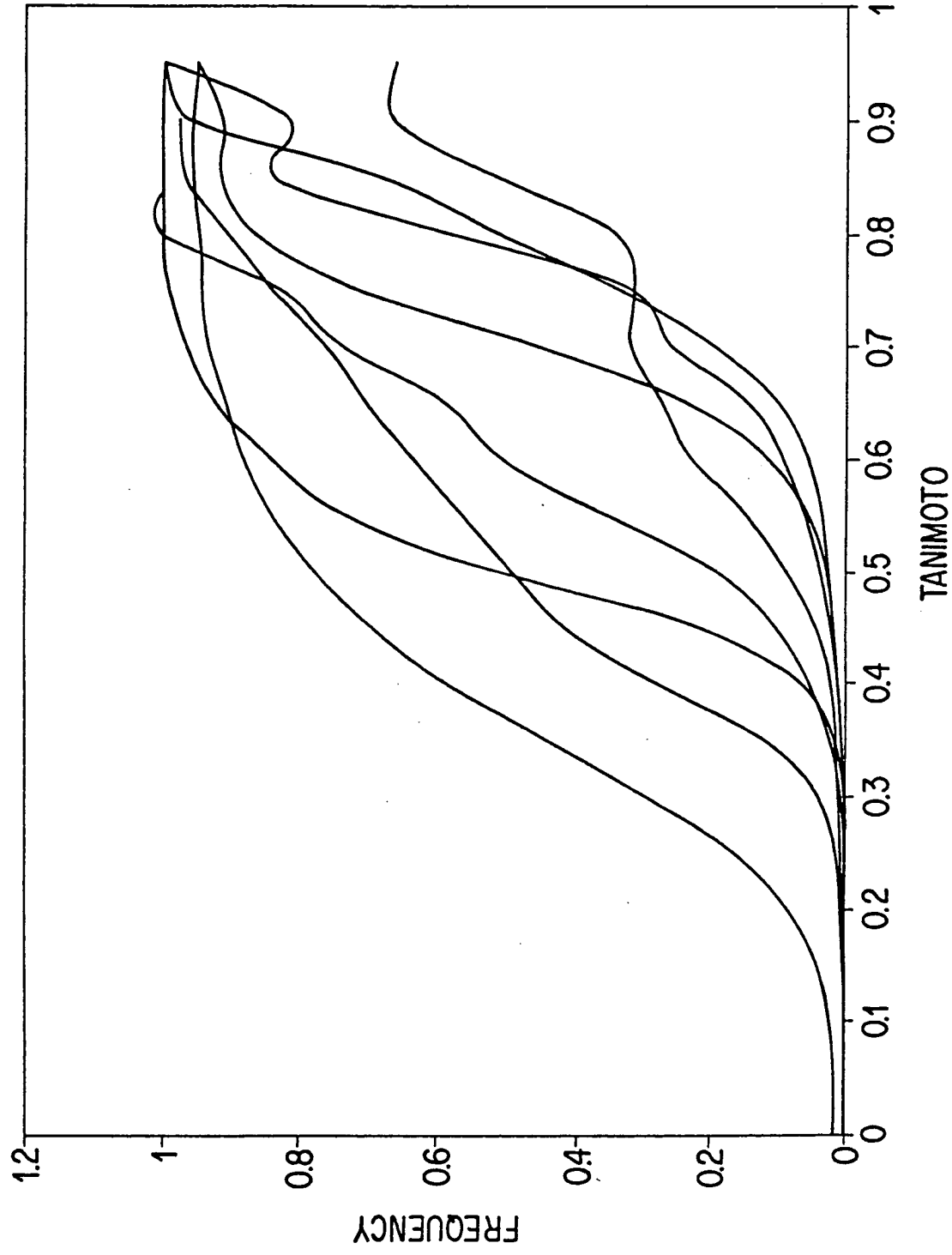


FIG. 9(b)

FOUO 3029260

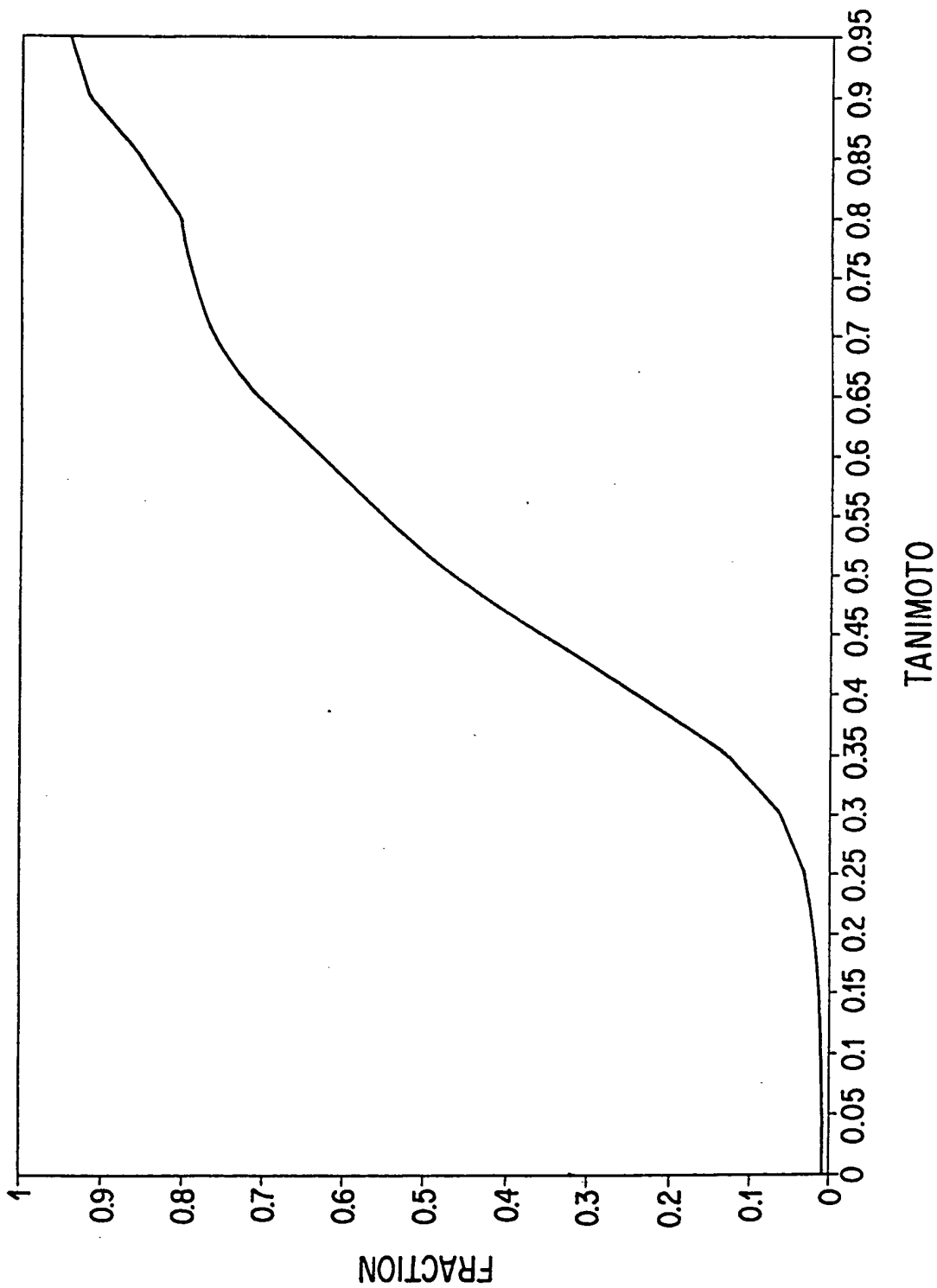


FIG. 9(c)

TOPICAL 3025260

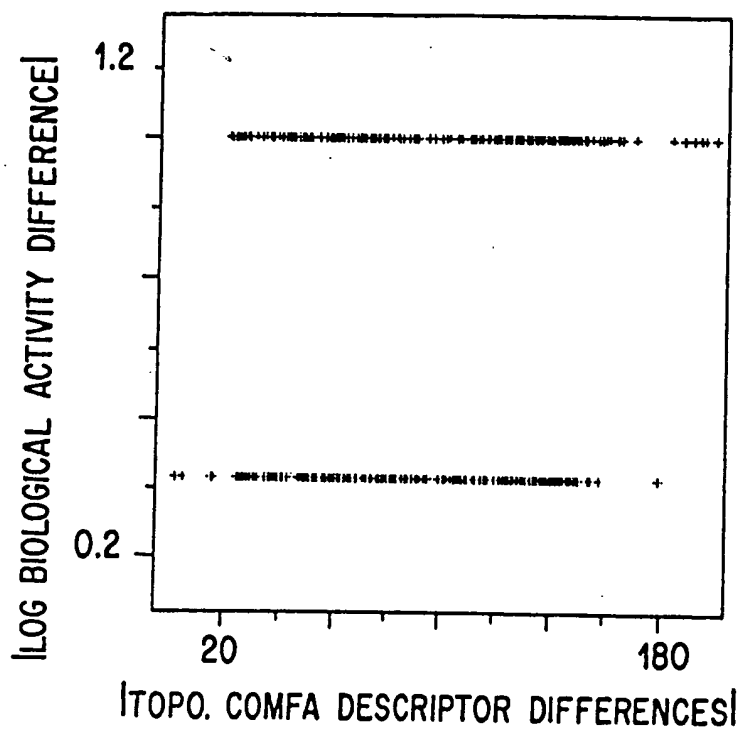


FIG. 10(a)

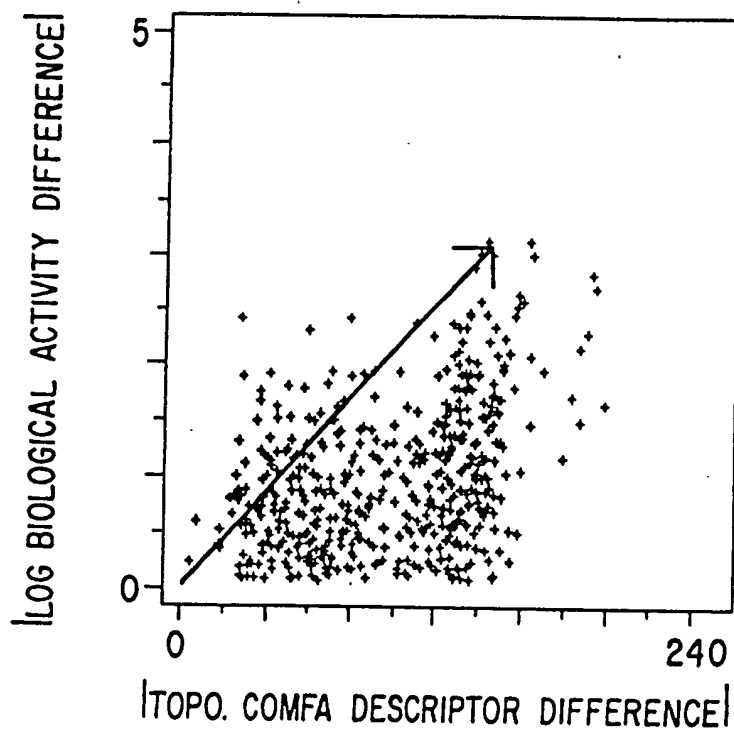


FIG. 10(b)

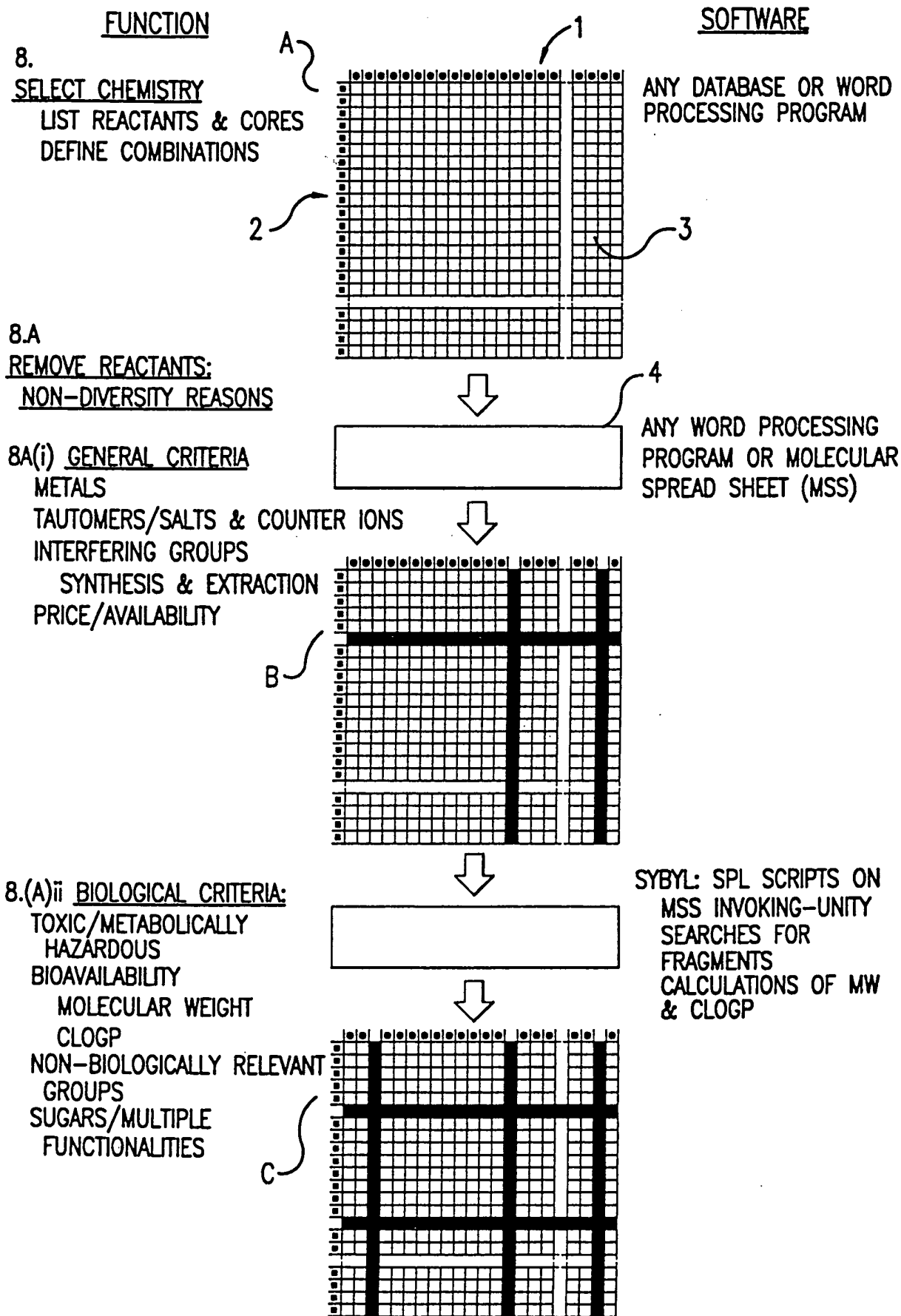


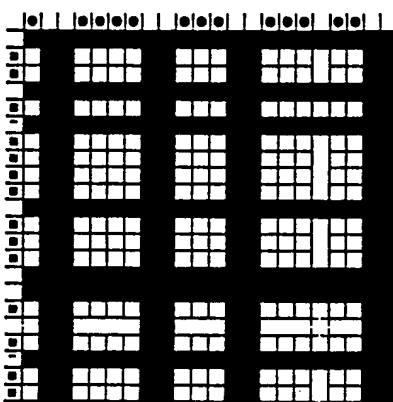
FIG.11(a)

8B

REMOVE NON-DIVERSE REACTANTS:

3D STRUCTURE GENERATION
 TOPOMERIC CONFORMER
 ALIGNMENT
 CoMFA FIELD GENERATION:
 HYDROGEN BOND FIELD
 GENERATION
 ROTATABLE BOND FIELD
 ATTENUATION
 CALCULATE FIELD
 DIFFERENCES
 CLUSTER
 REACTANT SELECTION FROM
 EACH CLUSTER

D



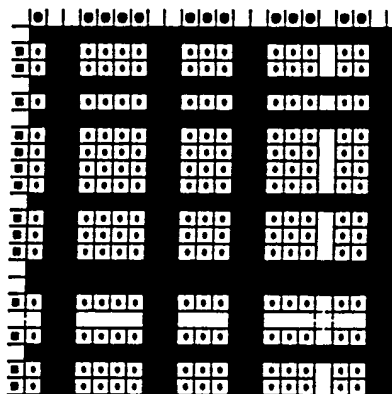
SYBYL: SELECTOR &
 CONCORD 3.2.1
 SPECIALIZED SOFTWARE:
 APPENDIX "A"
 (SYBYL: CoMFA
 STERIC & MSS)

SYBYL: HIERCHICAL
 CLUSTER - MSS
 SYLBL: MSS

8C

COMBINE REACTANTS TO BUILD PRODUCTS

E



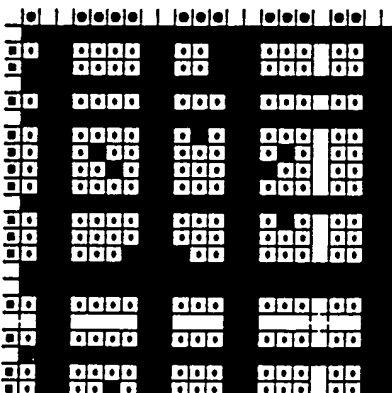
SYBYL: LEGION MSS

8D

REMOVE PRODUCTS:
NON-DIVERSITY REASONS

GENERAL CRITERIA:

F



SYBYL: SPL SCRIPTS
 ON MSS

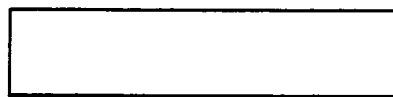
FIG.11(b)

FO5020" 8029260

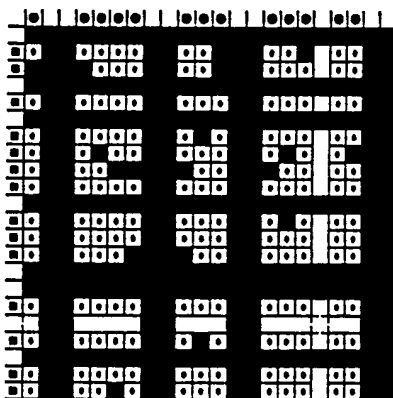
0976708.020504
FOUO 8029260

8D

BIOLOGICAL CRITERIA:
METABOLICALLY HAZARDOUS
BIOAVAILABILITY
MOLECULAR WEIGHT
CLOGP



G

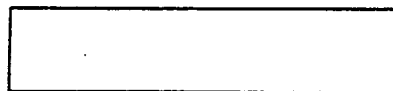


SYBYL: SPL SCRIPTS ON
MSS INVOKING -
UNITY SEARCHES FOR
FRAGMENTS
CALCULATIONS OF MW
& CLOGP

8E

REMOVE NON-DIVERSE
PRODUCTS:

GENERATE TANIMOTO
2D FINGERPRINTS
SAMPLE PRODUCTS:
EXCLUDE TAN ≥ 0.85



UNITY



H

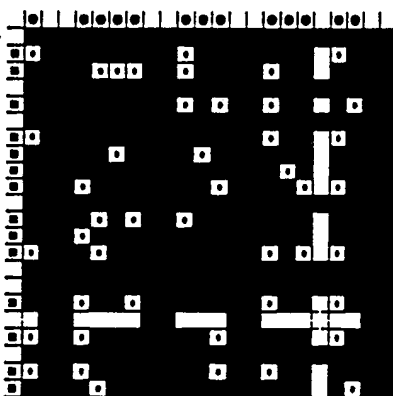
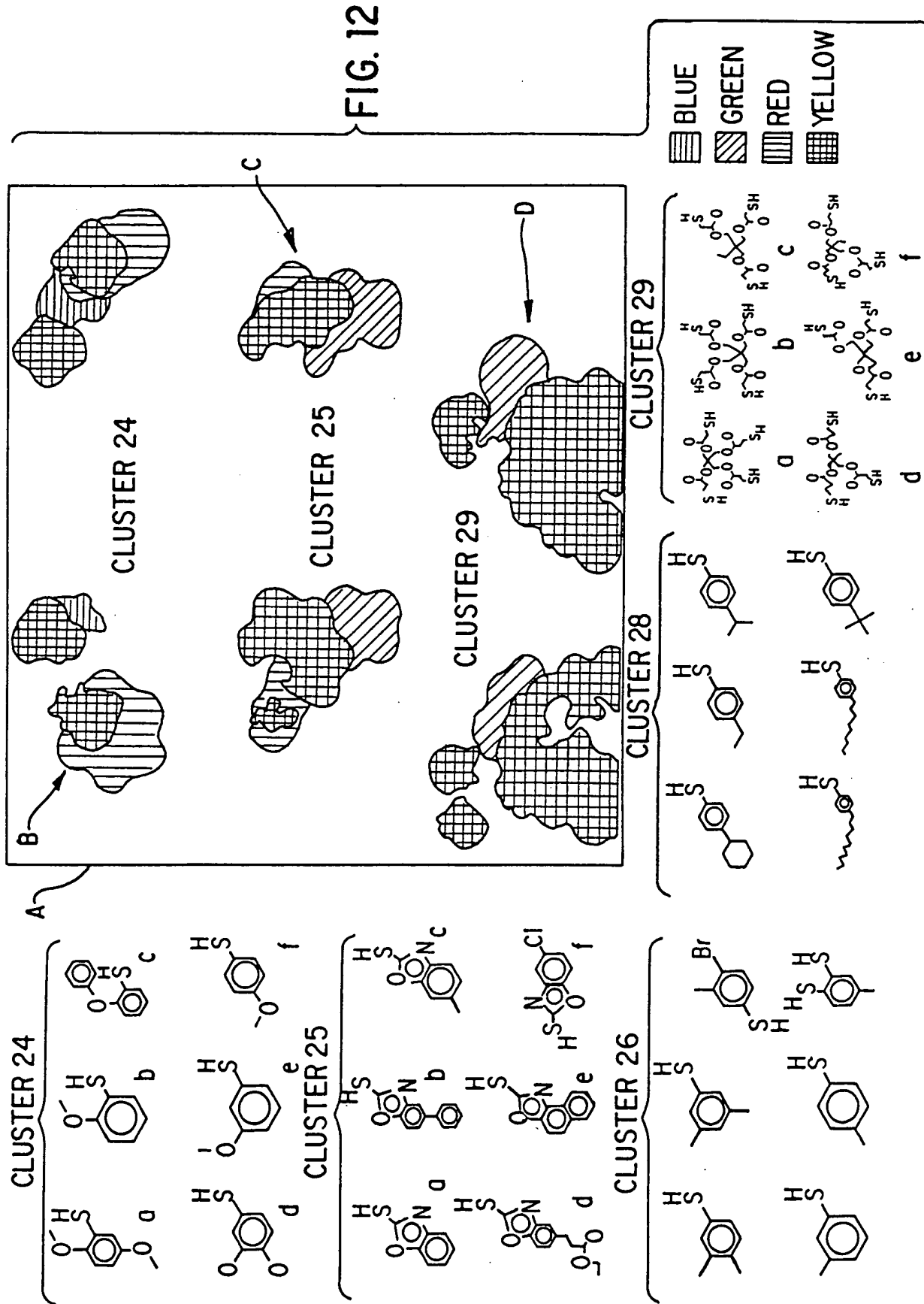


FIG.11(c)



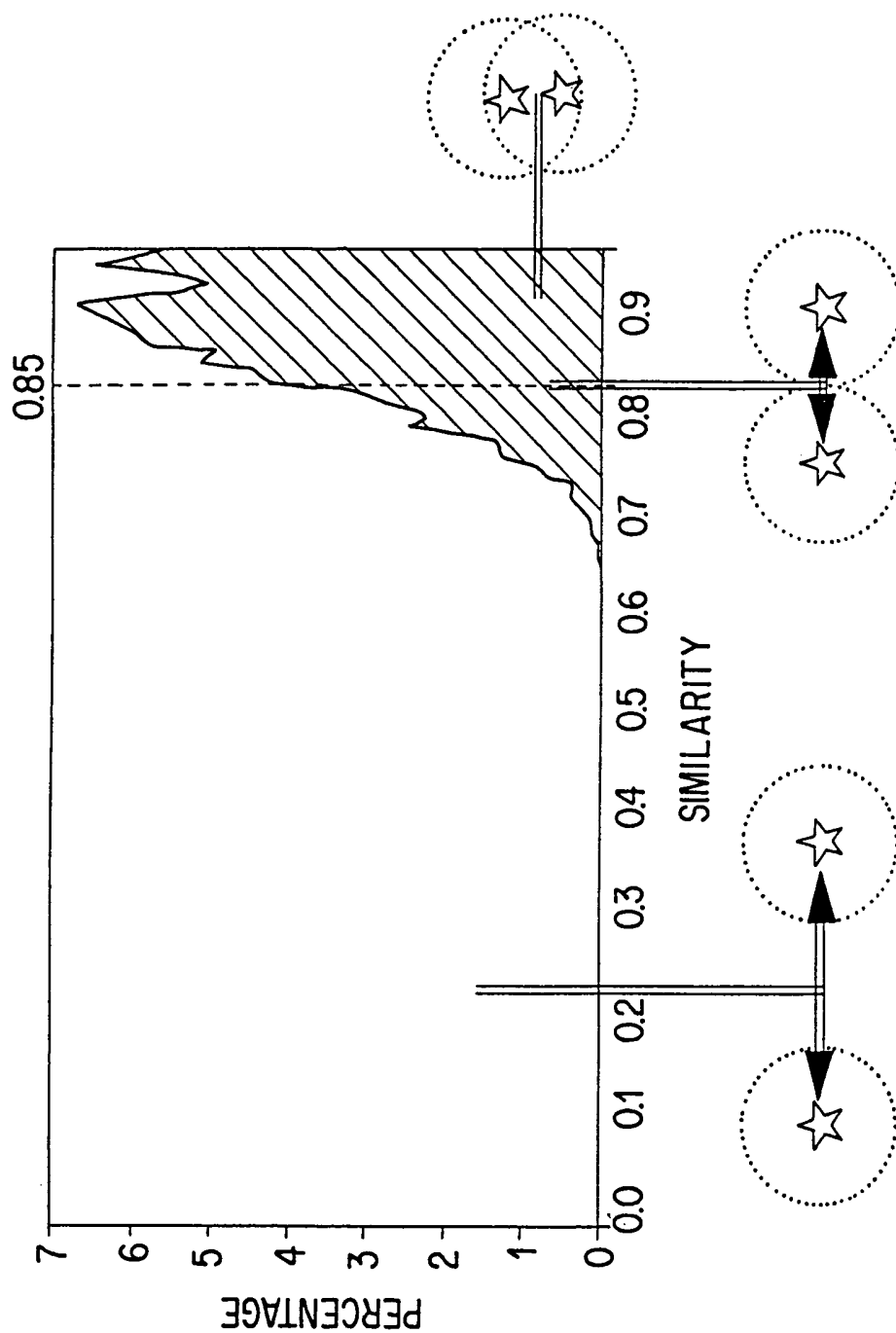


FIG.13

TOP SECRET 3329260

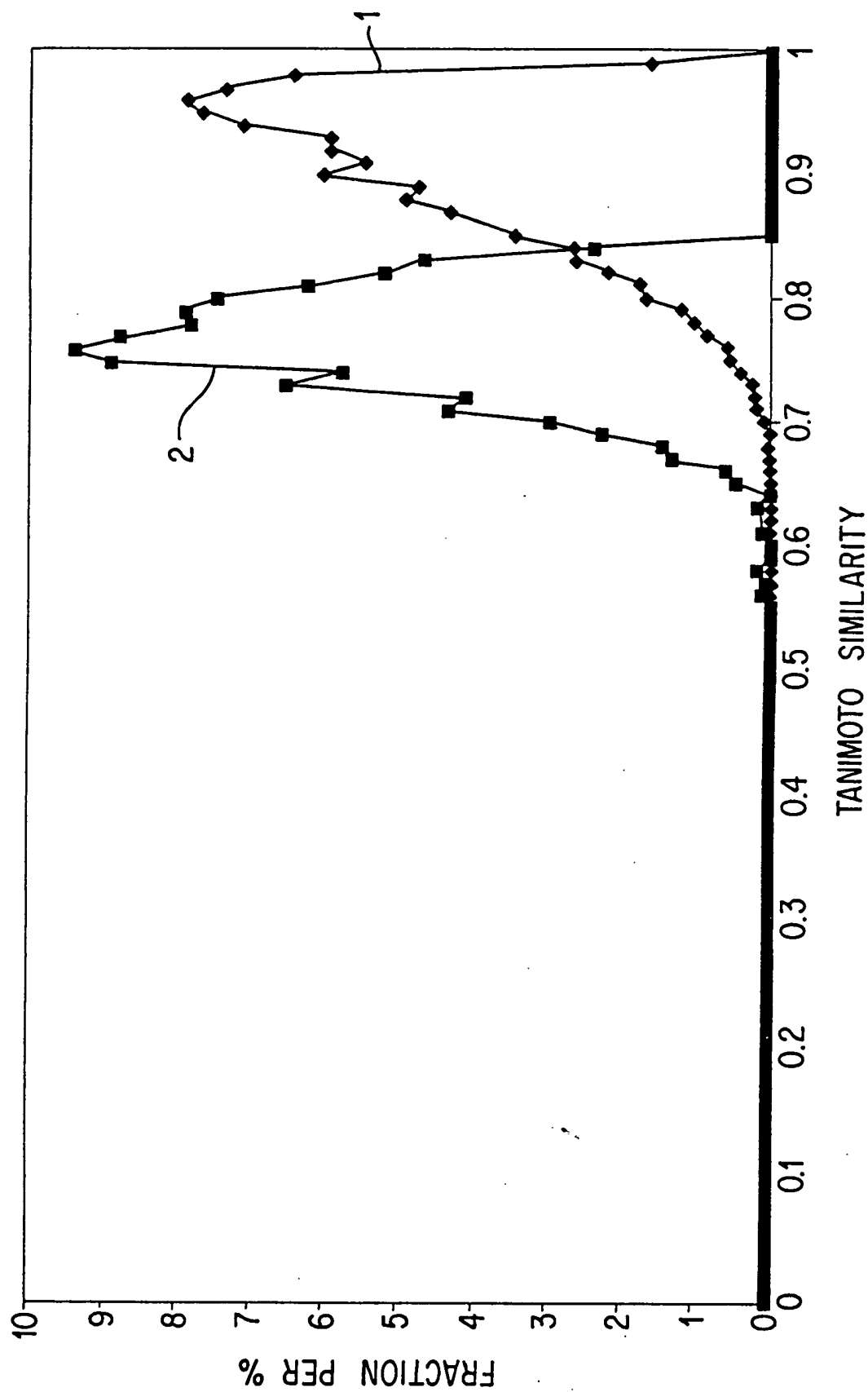


FIG.14

FO5020"8029260

↑
NO. OF COMPOUNDS

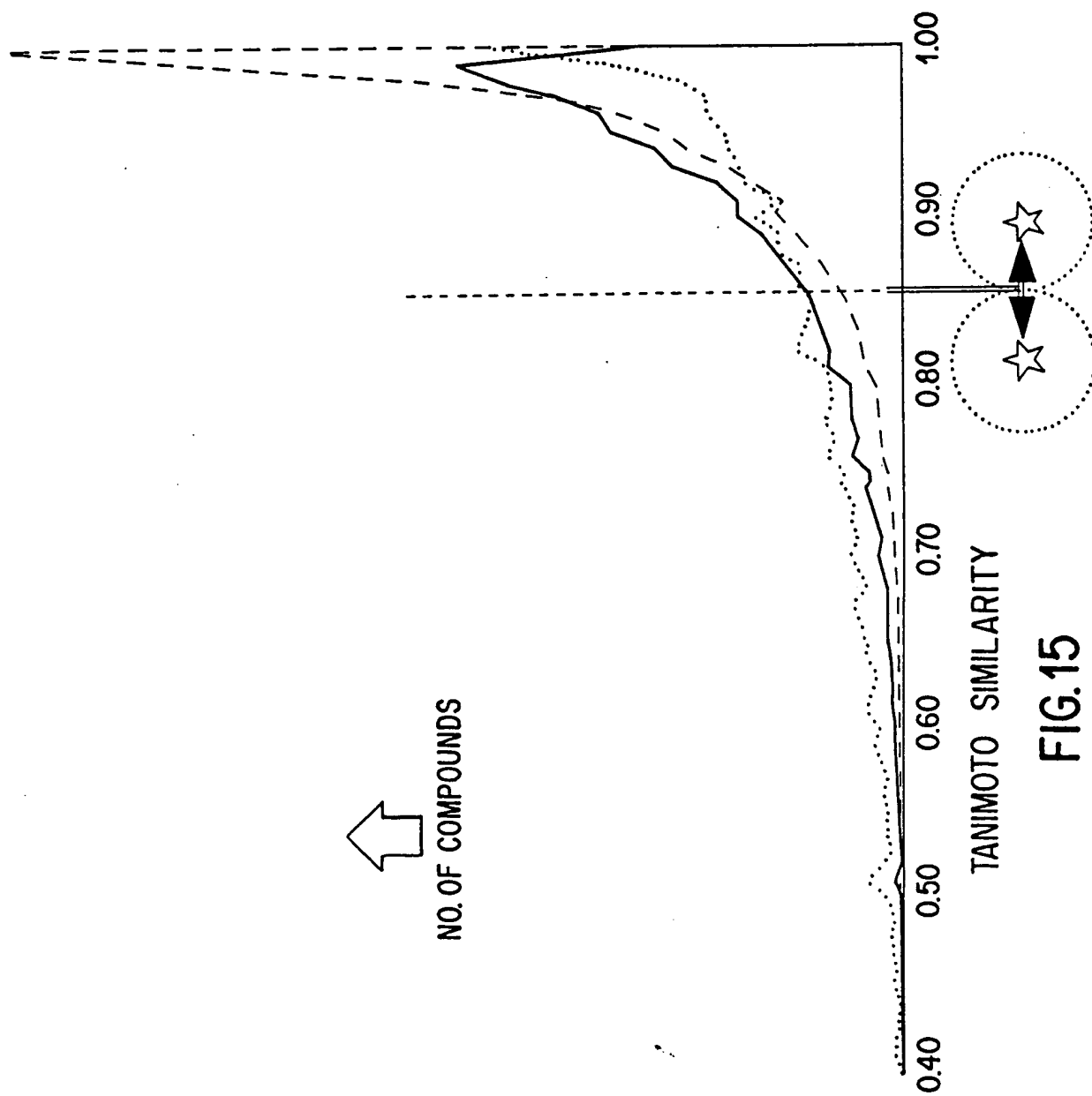


FIG.15